

# On generalized discrete PML optimized for propagative and evanescent waves

Vladimir Druskin,<sup>\*</sup> Murthy Guddati<sup>†</sup> Thomas Hagstrom,<sup>‡</sup>

## Abstract

We suggest a unified spectrally matched optimal grid approach for finite-difference and finite-element approximation of the PML. The new approach allows to combine optimal discrete absorption for both evanescent and propagative waves.

## 1 Introduction

We approximate the Neumann-to-Dirichlet (NtD) map of wave problem in unbounded domain. After Fourier transform we obtain,

$$u_{xx} - \lambda u = 0, \quad x \in [0, \infty] \quad (1)$$

and due to the infinity condition we are limited to outgoing wave solutions,

$$u = ce^{-\sqrt{\lambda}x}$$

satisfying NtD condition,

$$\frac{u}{u_x}\bigg|_{x=0} = -\frac{1}{\sqrt{\lambda}}. \quad (2)$$

Here  $\lambda = \kappa^2 - \omega^2$ , where  $\kappa$  and  $\omega$  are respectively (tangential) spacial and temporal frequencies. Also, (1) can be equivalently rewritten in the first order form as,

$$u_x = sv, \quad v_x = su, \quad (3)$$

where  $s = \sqrt{\lambda}$ . In terms of  $u$  and  $v$ , condition (2) can be equivalently rewritten as,

$$\frac{u}{v}\bigg|_{x=0} = -1. \quad (4)$$

The NtD can be numerically realized via rational approximation theory using several approaches [15, 10, 14, 11, 1, 12, 18, ?, etc]. In [14, 1] and [12, 18] this approximant was realized as respectively finite-difference (FD) and finite-element

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<sup>\*</sup>Schlumberger-Doll Research

<sup>†</sup>North Carolina State University

<sup>‡</sup>Southern Methodist University

(FE) discretization of an absorbing layer similar to well known Perfectly Matched Layer (PML) [6]. In particular, the FD scheme was designed as an optimal rational approximant separately for evanescent solutions corresponding to  $\lambda \geq 0$  [14] and propagative waves [1] corresponding to  $\lambda < 0$ , but not for the both types of the solutions simultaneously. On the other hand, FE approach is more flexible; while [12] focuses on propagative waves, it was shown in [18] that both propagative and evanescent waves can be treated simultaneously. Most recently, these FD and FE approximations are interpreted as special quadrature rules with complete wavefield approximation... [?].

In this paper, we show that simultaneous treatment of propagative and evanescent waves is possible not only in FE setting, but also in FD setting. The key to this observation is a recently-discovered equivalence between the FE and FD approaches for the two-sided problem. Utilizing this link, we present two alternative approaches to implement the NtD map and comment on their relative merits. Furthermore, utilizing Zolotarev approximation theory and complete wavefield approximation interpretation, we present an NtD map that is an optimal approximation for propagating as well as evanescent waves.

The outline of the paper is as follows. We start in section 2 with the overview of optimal rational approximation of the NtD map by considering both propagative and evanescent waves. Section 3 contains the description of FE and FD approximations of two-sided problems and the equivalence between them. In section 4, we consider rational approximation of the NtD map of the exterior problem and present FE and FD realizations. The implementation details in time domain and relative merits of the (or three) approaches are considered in section 5. Numerical examples are presented in section 6. Finally, section 7 concludes the paper with some closing remarks. **(where do we fit complete wavefield approximation of Tom?)**

## 2 Optimal Rational Approximation of NtD map for Propagative and Evanescent Waves

Let us for simplicity consider time-harmonic case with  $\omega = 1$  and consider time-dependent problems later. Let us present our rational approximant of  $-\lambda^{-1/2}$  as

$$-\lambda^{-1/2} \approx R(\lambda) = p(\lambda)/q(\lambda), \quad (5)$$

where  $p$  and  $q$  are polynomials of degrees  $K - 1$  and  $K$  respectively. Introducing a polynomial of degree  $N = 2K$  given by,

$$h(s) = sp(s^2) + q(s^2),$$

with  $s = \sqrt{\lambda}$ , we transform (5) to Newman function

$$R(s^2) = p(s^2)/q(s^2) = \frac{h(s) - h(-s)}{s[h(s) + h(-s)]} = \frac{-1 + h(s)/h(-s)}{s[1 + h(s)/h(-s)]}. \quad (6)$$

Then the relative error of the NtD map is approximately proportional to the reflection coefficient,

$$\frac{h(s)}{h(-s)}.$$

According to (4), the exact solution  $(u, v)$  of (3) is proportional to  $(1, -1)$ . In reality, due to the approximation error,  $(u, v)|_0 = c_1(1, -1) + c_2(1, 1)$ , and  $\frac{c_2}{c_1} = \frac{h(s)}{h(-s)}$ , i.e., the reflection coefficient is the ratio of the incoming and outgoing waves.

Minimization of  $\frac{h(s)}{h(-s)}$  on a real positive interval is the classical first Zolotarev problem solved in 1872. Zolotarev's solution was first applied to the optimal FD approximation of the NtD map for evanescent solutions in [14] and then to the approximation of propagative modes in [1]. The ABC for both propagative and evanescent waves should approximate the true NtD map on both negative  $[-1, \lambda_1]$  and positive  $[\lambda_2, \lambda_3]$  intervals. They respectively correspond to intervals  $S_p = [\sqrt{-1}, \sqrt{\lambda_1}]$  and  $S_e = [\sqrt{\lambda_2}, \sqrt{\lambda_3}]$  of variable  $s$ . The so called spectrally matched finite-difference scheme (a.k.a FD Gaussian spectral rule or optimal FD grid) [7, etc] allows arbitrary  $h(s)$ , but does not simultaneously treat propagative and evanescent waves. On the other hand, propagative and evanescent waves have been simultaneously treated using FE approximation in [18]. The specific approximation is based on linear FE approximation with midpoint integration [12], which is linked to special rational approximation [11] with

$$h(s) = t(s)^2, \quad (7)$$

where  $t$  is a polynomial of degree  $k$ .<sup>1</sup> Hence, considering the success in [18], we limit the current treatment to the restricted form of  $h$  in (7). With such restriction, minimization of  $\max_{s \in S_e \cup S_p} \left| \frac{h(s)}{h(-s)} \right|$  is equivalent to solving

$$\min_{\deg t \leq k} \max_{s \in S_e \cup S_p} \left| \frac{t(s)}{t(-s)} \right|. \quad (8)$$

It is well known that the necessary and sufficient conditions for optimality of a real rational approximant on a real interval is so-called the Equal Ripple Theorem (ERT) [16]. It says that the optimal error of  $[(K-1)/K]$  approximant has  $2k - 1$  zeros and  $2k$  equal absolute value alternating extrema on the interval of optimality. Generally, there is no similar result for complex rational approximation [17]. Here, instead of minimizing (8), we construct an approximant based on classical Zolotarev results. We hope that its error is close to (8).

If  $t = t_e t_p$ ,  $\deg t_e = l < k$ ,  $\deg t_p = k - l$ , where  $t_e$  and  $t_p$  have respectively (non-coinciding) roots on  $S_e$  and  $S_p$ , then  $\left| \frac{t(s)}{t(-s)} \right|$  has  $2k + 1$  maxima on  $S_p \cup S_e$ . Moreover,  $\left| \frac{t_e(s)}{t_e(-s)} \right| = 1$  on  $S_p$  and  $\left| \frac{t_p(s)}{t_p(-s)} \right| = 1$  on  $S_e$ , which implies that,

$$\max_{S_e} \left| \frac{t(s)}{t(-s)} \right| = \max_{S_e} \left| \frac{t_e(s)}{t_e(-s)} \right|,$$

and

$$\max_{S_p} \left| \frac{t(s)}{t(-s)} \right| = \max_{S_p} \left| \frac{t_p(s)}{t_p(-s)} \right|.$$

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<sup>1</sup> However, as it will be shown in the Section 4, simultaneous treatment of propagating and evanescent waves is even possible with more general  $h(s)$ , if the FD approach is used.

Thus, we can take as  $t_e$  and  $t_p$  as the classical optimal Zolotarev approximants on  $S_e$  and  $S_p$  respectively, and obtain the quality of the total approximation the same as the one of the separate problems.

The remaining question is: can the constructed approximant be optimal in global sense, or, at least, how close is its error to (8). Obviously,  $\max_{S_p} \left| \frac{t(s)}{t(-s)} \right|$  and  $\max_{S_e} \left| \frac{t(s)}{t(-s)} \right|$  may be different. Varying  $l$  one can equate  $\max_{S_p} \left| \frac{t(s)}{t(-s)} \right|$  and  $\max_{S_e} \left| \frac{t(s)}{t(-s)} \right|$  for a countable set of arrays  $\lambda_1, \lambda_2, \lambda_3$ .

Here we conjecture that the ERT can be extended to the first Zolotarev problem on two intervals in  $C$  in the following way.

**Conjecture 1:** Let  $t_e(s)/t_e(-s)$  and  $t_p(s)/t_p(-s)$  be the solutions of the Zolotarev problems on  $S_e$  and  $S_p$  respectively.

1. There are infinitely many arrays  $\lambda_1, \lambda_2, \lambda_3$  for which there exists  $l$ , such that

$$\max_{S_e} \left| \frac{t_e(s)}{t_e(-s)} \right| = \max_{S_p} \left| \frac{t_p(s)}{t_p(-s)} \right|. \quad (9)$$

2. If (9) is valid, then  $t = t_e t_p$  solves (8).

Results of [?] indicate that, if (9) is valid, then at least the approximant is optimal in the Cauchy–Hadamard sense. Generally, it is always possible to find  $l$  such that  $\max_{S_p} \left| \frac{t(s)}{t(-s)} \right|$  and  $\max_{S_e} \left| \frac{t(s)}{t(-s)} \right|$  are of the same order, in which case, it is natural to assume that the approximation error will be of the order of (8).

### 3 Equivalence of FE and FD Approximations for Two-sided Problems

While the emphasis of this paper is on the approximation of the one-sided problem on  $[0, \infty)$ , in this section, we consider the two-sided problem on  $[0, 1]$  and show that there exist equivalence between spectrally matched FD grids and midpoint integrated linear FE mesh. We then utilize these results in Section 4 to construct an effective NtD map for the one-sided problem on  $[0, \infty)$ .

#### 3.1 Continuum problem

**QUESTION:** You have used \* for many row vectors and matrices. Should we be just using transpose? [decide later](#).

Let us consider eq. (3) on  $[0, 1]$ , and define the two-sided DtN map as matrix-valued function  $F(s) \in C^{2 \times 2}$

$$F(s)u_b = v_b,$$

where  $u_b = [u(0), u(1)]^*$ ,  $v_b = [v(0), -v(1)]^*$ . It is easy to see that  $(u, v)$  is a linear combination of,

$$(e^{\pm sx}, \pm e^{\pm sx}),$$

and simple computation shows that,

$$F(s) = \frac{1}{\sinh(s)} \begin{bmatrix} \cosh(s) & -1 \\ -1 & \cosh(s) \end{bmatrix} = Z \begin{bmatrix} \tanh(s/2) & 0 \\ 0 & \coth(s/2) \end{bmatrix} Z^*, \quad (10)$$

where  $Z$  is an orthogonal matrix

$$Z = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}.$$

Similarly, we define propagator operator from left to right as matrix-valued function  $G(s) \in C^{2 \times 2}$   $G(s)w(0) = w(1)$ , where  $w = (u, v)^*$  and from (10) we obtain

$$G = \begin{bmatrix} \cosh(s) & \sinh(s) \\ \sinh(s) & \cosh(s) \end{bmatrix} = Z \begin{bmatrix} \exp(s) & 0 \\ 0 & \exp(-s) \end{bmatrix} Z^*. \quad (11)$$

### 3.2 Discrete problem: linear FE mesh with midpoint rule

It was shown in [12] that the discretization of the original second-order from in (1) with midpoint-integrated linear FE mesh would lead to exponential convergence of the NtD map. Furthermore, it was shown in [13] that such a FE discretization is equivalent to Crank-Nicholson discretization of the first order form (3), i.e.

$$\frac{u_{i+1} - u_i}{l_i} = s \frac{v_{i+1} + v_i}{2}, \quad \frac{v_{i+1} - v_i}{l_i} = s \frac{u_{i+1} + u_i}{2}, \quad i = 1, \dots, n. \quad (12)$$

where  $l_i$ ,  $i = 1, \dots, n$  are the FE lengths with  $\sum_{i=1}^n l_i = 1$ . It can be easily verified that  $(u_j, v_j)$ ,  $j = 1, \dots, n$ , is a linear combination of

$$\left( \prod_{i=1}^j \frac{1 \pm l_i s/2}{1 \mp l_i s/2}, \pm \prod_{i=1}^j \frac{1 \pm l_i s/2}{1 \mp l_i s/2} \right).$$

Comparing the above (approximate) solution with the exact solution and noting that  $\sum_{i=1}^n l_i = 1$ , the FE solution approximates the exponential as

$$\exp(s) \approx \exp(s) = t(-s)/t(s),$$

where

$$t(s) = \prod_{i=1}^n (1 - l_i s/2),$$

Assuming

$$u(0) = u_1, \quad u(1) = u_n, \quad v(0) \approx v_1, \quad v(1) \approx v_n, \quad (13)$$

we can compute the approximate NtD map as,

$$\tilde{F}(s) = \frac{1}{\sinh(s)} \begin{bmatrix} \cosh(s) & -1 \\ -1 & \cosh(s) \end{bmatrix} = Z \begin{bmatrix} \tanh(s/2) & 0 \\ 0 & \coth(s/2) \end{bmatrix} Z^*. \quad (14)$$

Here,

$$\sinh(s) = \frac{\exp(s) - \exp(-s)}{2} \approx \sinh(s), \quad \cosh(s) = \frac{\exp(s) + \exp(-s)}{2} \approx \cosh(s),$$

$$\tanh(s/2) = \frac{t(s) - t(-s)}{t(s) + t(-s)} \approx \tanh(s/2), \quad \coth(s) = 1/\tanh(s) \approx \coth(s).$$

Similarly, the discrete propagator from left to right matrix can be computed as

$$\tilde{G} = \begin{bmatrix} \cosh(s) & \sinh(s) \\ \sinh(s) & \cosh(s) \end{bmatrix} = Z \begin{bmatrix} \exp(s) & 0 \\ 0 & \exp(-s) \end{bmatrix} Z^*. \quad (15)$$

Vectors  $\frac{1}{\sqrt{2}}(1, \pm 1)$  are the eigenvectors of  $\tilde{G}$ , so it has so called fixed point property, i.e., if  $u(0)/v(0) = \pm 1$  then  $u(1)/v(1) = \pm 1$  and vice versa. This implies that, if exact half-space BC (4) is applied at  $x = 0$ , it will be also valid at  $x = 1$  regardless of the accuracy of the FE approximation. In other words, adding an FE-discretized interval to a half-space does not alter the NtD map of the half-space. Furthermore, it was shown in [12] that adding a midpoint-integrated finite element to an approximate half-space can only decrease the approximation error in the NtD map. This property was used in [18] to enhance the approximation, originally designed for propagative waves, to simultaneously absorb evanescent waves.

### 3.3 Discrete Problem: spectrally matched finite-difference grids

It was shown in [] that one-sided, two-point BVP can be solved with staggered FD method with exponential convergence at the end points. The main idea was to link the staggered FD approximation to rational approximation of the exact NtD map and optimizing the resulting approximation using Zolotarev theory. This method was later extended to the solution of the two-sided problems by splitting the solution into odd and even parts and solving two one-sided problems on half-intervals using dual grids. Formerly called optimal FD grids, the basic idea of spectrally matched FD grids is summarized below.

Let us introduce the FD grid steps  $\hat{h}_i, h_i, i = 1, \dots, k$ . We split the DtN map into odd and even parts and compute each of them using a FD scheme on half interval. The odd and even problems can respectively be written in mutually dual form as:

$$\frac{u_{i+1}^o - u_i^o}{h_i} = sv_i^o, \quad \frac{v_i^o - v_{i-1}^o}{\hat{h}_i} = su_i^o, \quad i = 1, \dots, k, \quad u_{k+1} = 0, \quad (16)$$

$$\frac{u_{i+1}^e - u_i^e}{\hat{h}_i} = sv_i^e, \quad \frac{v_i^e - v_{i-1}^e}{h_i} = su_i^e, \quad i = 1, \dots, k, \quad v_{k+1} = 0.$$

It is known [7] that,

$$\frac{u_1^o}{v_1^o} = \frac{v_1^e}{u_1^e} = f_k(s) = \frac{1}{\hat{h}_1 s + \frac{1}{h_1 s + \frac{1}{\hat{h}_2 s + \dots \frac{1}{h_{k-1} s + \frac{1}{\hat{h}_k s + \frac{1}{h_k s}}}}}}. \quad (17)$$

Combining odd and even parts we obtain,

$$u(0) = u_1^e + u_1^o, \quad u(1) = u_1^e - u_1^o, \quad v_1^e \approx \frac{v(0) + v(1)}{2}, \quad v_1^o \approx \frac{v(0) - v(1)}{2}, \quad (18)$$

and the FD-NtD as

$$\hat{F} = Z \begin{bmatrix} f_k & 0 \\ 0 & 1/f_k \end{bmatrix} Z^*. \quad (19)$$

Construction of spectrally matched grids involves a reverse procedure. First, rational approximation theory is used to obtain  $f_k$  that approximates the NtD map. The resulting rational function is then used in (17) to compute the grid steps  $\hat{h}_i, h_i$  using simple \*\*\*\* algorithm []. \*\*\*\* algorithm also constructively shows that any  $[2k-1/2k]$  rational function can be converted into an equivalent FD grid.

### 3.4 Equivalence of discrete problems

In this section, we show that if the number of finite elements are chosen to be even ( $n = 2k$ ), the approximate NtD maps from FE and FD grids are equivalent.

**Lemma 1:** For any set of parameters  $l_i \in C$ ,  $l = 1, \dots, 2k$  there exist parameters  $\hat{h}_i, h_i \in C \cup \infty$ ,  $l = 1, \dots, k$ , such that

$$f(s) \equiv \tanh(s/2) \quad (20)$$

and vice versa.

*Proof.* For any set of parameters  $\hat{h}_i, h_i \in C \cup \infty$  there exist polynomials  $p$  and  $q$  (at most) degree  $k - 1$  and  $k$  respectively, such that the continued fraction expansion (17) can be presented as

$$f_k = \frac{sp(s^2)}{q(s^2)},$$

and vice versa. Equating numerator and denominator of  $f_k$  and  $\tanh$  we equivalently transform (20) to polynomial identities

$$sp(s^2) \equiv t(s) - t(-s), \quad q(s^2) \equiv t(s) + t(-s). \quad (21)$$

Since  $p$ ,  $q$  and  $t$  can be arbitrary polynomials of degree  $k - 1$ ,  $k$  and  $2k$  respectively, then for any  $p, q$  there is  $t$  satisfying (21) and vice versa. **(Aren't these different p**

and  $q$ ? If so, it is important not to confuse the polynomials  $p$  and  $q$  with the polynomials in the second equation in section 2. Should be rename these as  $\tilde{p}$  and  $\tilde{q}$ ? Agree, will do it later  $\square$

From the lemma, (14) and (19), we obtain the following result about equivalence of the FE and FD DtN maps.

**Proposition 1:** If (20) is valid, then

$$\tilde{F}(s) \equiv \hat{F}(s).$$

Formula (21) can be used for computing the equivalent FE from the FD and vice versa.

If the DtN maps are identical, then formula (15) can also be used for computing the propagator matrix for the FD approximation.

If  $\exp(s)$  matches  $\exp(s)$  in  $n$  non-coinciding frequencies, then  $f_k$  matches  $\tanh(s)$  at the same frequencies, and  $f_k$  is Stieltjes function,  $h_i, \hat{h}_i$  are real positive, and the problem becomes Hermitian.

## 4 Approximation of exterior problems

Let a discretized interval  $\Omega_1 = [x_-, x_+]$  have the propagator matrix (from left to right),

$$\tilde{\mathcal{G}} = \begin{bmatrix} \exp_1(s) & 0 \\ 0 & \exp_1(-s) \end{bmatrix}$$

in the spectral coordinates, where  $\exp_1(s) = t_1(-s)/t_1(s)$  defined as in the previous section. First, let us impose the reflection coefficient  $h_2(s)/h_2(-s)$  at  $x_+$ , i.e., at the right boundary any nontrivial solution can be represented as  $w(x_+) = [ch_2(s), -ch_2(-s)]^*$  in the spectral coordinates, where  $c \neq 0$  is an arbitrary constant. Then the reflection coefficient at the left boundary will be the ratio of the components of  $w(x_-) = \tilde{\mathcal{G}}^{-1}w(x_+)$ . That is,

$$\exp_1(-s)^2 \frac{h_2(s)}{h_2(-s)} = \frac{t_1(s)^2}{t_1(-s)^2} \frac{h_2(s)}{h_2(-s)}. \quad (22)$$

If we impose the Dirichlet condition at the right boundary of  $\Omega_1$ , which corresponds to  $h_2(s) = 1$ , then the reflection coefficient will be  $\frac{t_1(s)^2}{t_1(-s)^2}$ . Let us now assume that we have a connected interval  $\Omega = \Omega_1 \cup \Omega_2$  with the Dirichlet condition at the right boundary ( $\Omega_2$  is assumed to be on the right), and  $\frac{h_2(s)}{h_2(-s)}$  is the reflection coefficient of  $\Omega_2$ . Then (22) would yield the reflection coefficient of  $\Omega$  that is just the product of the reflection coefficients of the two subdomains.

Now, let us assume, that we use the discrete problem in  $\Omega$  for the approximation of (4), i.e.,  $h(s)$  from (6) can be presented as  $h(s) = t_1(s)^2 h_2(s)$ . If we set  $h_1 \equiv t_1^2$  and  $t_1 \equiv t_e$  and  $t_2 \equiv t_p$ , then the reflection coefficient of  $\Omega$  will be identical to the one discussed in Section 2. However, Dirichlet condition on the right of  $\Omega_2$  makes it a one-sided problem, and it is not necessary to restrict to the two-sided approximation in the previous section. In fact, the original FD optimal grids are optimized for



the one-sided problems and can be used effectively for  $\Omega_2$ . This approximation is equivalent to the odd part of the FD approximation (16), i.e.,

$$\frac{u_{i+1}^o - u_i^o}{h_i} = sv_i^o, \quad \frac{v_i^o - v_{i-1}^o}{\hat{h}_i} = su_i^o, \quad i = 1, \dots, k, \quad u_{k+1} = 0.$$

Then  $h_2$  can be obtained from the equality  $f_k(s) = \frac{h_2(s) - h_2(-s)}{h_2(s) + h_2(-s)}$ , i.e., it can be an arbitrary polynomial of degree  $2k$ . {

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